

# **A FUNDAMENTAL EQUATION FOR THE CALCULATION OF THE THERMODYNAMIC PROPERTIES OF ETHANOL<sup>1</sup>**

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## ABSTRACT

A formulation for the thermodynamic properties of ethanol ( $\text{C}_2\text{H}_5\text{OH}$ ) in the liquid, vapor, and saturation states is presented. The formulation is valid for single-phase and saturation states from 250 K to 650 K at pressures up to 280 MPa. The formulation includes a fundamental equation and ancillary functions for the estimation of saturation properties. The experimental data used to determine the fundamental equation include pressure-density-temperature, isochoric heat capacity, speed of sound, and vapor pressure. Saturation values computed from the ancillary functions were used to ensure thermodynamic consistency at the vapor-liquid phase boundary. Comparisons between experimental data and values computed using the fundamental equation are given to verify the uncertainties in the calculated properties. The formulation presented may be used to compute densities to within  $\pm 0.2\%$ , heat capacities to within  $\pm 3\%$  and speed of sound to within  $\pm 1\%$ . Saturation values of the vapor pressure and saturation densities are represented to within  $\pm 0.5\%$ , except near the critical point.

## 1. INTRODUCTION

Ethanol ( $\text{C}_2\text{H}_5\text{OH}$ ) is used in many industrial applications. In recent years, ethanol has received significant consideration as a renewable bio-fuel that can help reduce dependence on fossil fuels. The design of engineering systems utilizing ethanol requires accurate knowledge of the thermodynamic properties of the fluid. This paper presents a formulation for ethanol that includes a fundamental equation for the calculation of thermodynamic properties, and supporting ancillary functions.

The formulation presented for ethanol is valid in the single-phase regions from 250 K to 650 K at pressures to 280 MPa. Ancillary functions for the vapor pressure, saturated liquid density, and saturated vapor density are provided as estimating functions for iterative computer programs which are used to calculate the thermodynamic properties of ethanol with various pairs of independent variables. Saturation properties can be computed by invoking the Maxwell Criterion or by simultaneous solution of the vapor pressure equation with the fundamental equation. The method of simultaneous solution produces values that are not thermodynamically consistent. However, the computed saturation properties are within  $\pm 0.5\%$  of the Maxwell Criterion values, except near the critical point.

## 2. EXPERIMENTAL DATA FOR ETHANOL

The available experimental data for ethanol are summarized in Tables I and II. Table I lists the single-phase data, and Table II shows data for the saturation properties and the ideal gas heat capacity. Not all of the data listed in Tables I and II were used in the development of the formulation. However, all data listed in Tables I and II are compared to values calculated with the formulation. The data used to develop the formulation are indicated with asterisks in Tables I and II. Also listed in Tables I and II are columns that indicate the absolute average deviation (AAD) between values computed by a formulation and experimental data. The AAD for any property,  $X$ , is defined as,

$$AAD = \frac{1}{n} \sum_{i=1}^n |(\% \Delta X)_i| \quad (1)$$

where  $\% \Delta X$  represents the percent deviation between the calculated property and the experimental data, defined by,

$$\% \Delta X = 100 \left( \frac{X_{data} - X_{calc}}{X_{data}} \right) \quad (2)$$

In the formulation presented here, the critical parameters of the fluid are used as reducing parameters. The critical parameters were selected after evaluating the existing reported values. There is a significant range in the measured critical parameters mostly attributed to a wide variation in ethanol purity (from 90% to 99.99%). One of the reasons for this variation in purity is ethanol's high affinity for water. If the sample is not highly purified, the data will be compromised by the presence of the water. In addition, if the experimental apparatus contains traces of water vapor, a highly purified sample will become contaminated and render the data uncertain. With this in mind, the measured values of critical temperature and pressure of Ambrose et al. [28], and the critical density predicted with a corresponding states method of Ambrose and Walton [42] were used to define the critical point for this work,

$$P_c = 6.148 \text{ MPa}, \rho_c = 5.991 \text{ mol} \cdot \text{dm}^{-3}, \text{ and } T_c = 513.9 \text{ K}$$

Other constants used required by the formulation are the molar mass of ethanol,  $46.06904 \text{ g} \cdot \text{mol}^{-1}$ , and the universal gas constant,  $8.314472 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$  after Mohr and Taylor [43].

### 3. ANCILLARY FUNCTIONS FOR ETHANOL

Ancillary functions for the vapor pressure, saturated liquid density, and saturated vapor density have been developed. These equations are not required for property calculation. However, they do provide excellent estimates for the iterative solution of

calculations requiring the application of the Maxwell Criterion. The ancillary equations were developed using the selected experimental data designated with asterisks in Table II.

The vapor pressure of ethanol is given by,

$$\ln \frac{P}{P_c} = \frac{T_c}{T} (a_1 \theta^{1/2} + a_2 \theta + a_3 \theta^3 + a_4 \theta^{1/2}) \quad (3)$$

where  $a_1 = -0.0514770863682$ ,  $a_2 = -8.27075196981$ ,  $a_3 = -5.49245388577$ ,  $a_4 = 5.64828891406$ , and  $\theta = 1 - T/T_c$ . This equation can be used to predict vapor pressure values for ethanol to within  $\pm 0.4\%$ .

The saturated liquid density of ethanol is represented by,

$$\frac{\rho'}{\rho_c} = 1 + b_1 \theta^{1/3} + b_2 \theta + b_3 \theta^{5/3} + b_4 \theta^2 + b_5 \theta^{8/3} \quad (4)$$

where  $b_1 = 2.22194636037$ ,  $b_2 = -0.0469267553094$ ,  $b_3 = 10.3035666311$ ,  $b_4 = -17.2304684516$ ,  $b_5 = 8.23564165285$ , and  $\theta$  is defined as in Eq. (3). Eq. (4) represents the selected experimental data to within  $\pm 0.2\%$

There is little reliable data for the saturated vapor density of ethanol. The data of Fiock et al. [38] were used in the limited range from 273 to 393 K. The final ancillary equation for the saturated vapor density was determined by fitting data from the intersection of the equation of state with the vapor pressure equation. The resulting equation for the saturated vapor density is,

$$\ln \left( \frac{\rho''}{\rho_c} \right) = c_1 \theta^{2/3} + c_2 \theta^{5/3} + c_3 \theta^{10/3} + c_4 \theta^{16/3} \quad (5)$$

where  $c_1 = -8.35647816638$ ,  $c_2 = -2.38721859682$ ,  $c_3 = -39.6946441837$ , and  $c_4 = -9.99133502692$ , and  $\theta$  is defined as in Eq. (3).

#### 4. THE FUNDAMENTAL EQUATION FOR ETHANOL

The functional form of the fundamental equation used for this formulation was developed by Jacobsen et al. [44]. This equation is a potential function explicit in dimensionless Helmholtz energy with reduced density and reciprocal reduced temperature as independent variables. The form of the fundamental equation is,

$$\alpha(\delta, \tau) = \alpha^0(\delta, \tau) + \bar{\alpha}(\delta, \tau) \quad (6)$$

where  $\delta = \rho/\rho_c$ ,  $\tau = T_c/T$ , and  $\alpha = a/RT$ . The superscript '0' signifies the ideal gas contribution to the dimensionless Helmholtz energy, and the over bar is the real fluid residual.

The ideal gas reduced Helmholtz energy can be derived from fundamental thermodynamic relationships for the ideal gas, and is given by,

$$\alpha^0(\delta, \tau) = \frac{h_0^0 \tau}{RT_c} - \frac{s_0^0}{R} - 1 + \ln \frac{\delta \tau_0}{\delta_0 \tau} + \frac{\tau}{R} \int_{\tau_0}^{\tau} \frac{c_p^0}{\tau^2} d\tau + \frac{1}{R} \int_{\tau_0}^{\tau} \frac{c_p^0}{\tau} d\tau \quad (7)$$

where  $\delta_0 = \rho_0/\rho_c$  and  $\tau_0 = T_c/T_0$ . The value of  $\rho_0$  is determined from the ideal gas density at  $T_0$  and  $P_0$ . The reference values are arbitrary. In this work, the values of  $P_0 = 0.001$  MPa and  $T_0 = 273.15$  K were adopted. The reference enthalpy and entropy values are also arbitrary, and were computed to eliminate negative property values within the limits of the fundamental equation. The resulting values are,  $h_0^0 = 45800$  J·mol<sup>-1</sup> and  $s_0^0 = 180$  J·mol<sup>-1</sup>·K<sup>-1</sup>.

In order to complete the ideal gas calculation in Eq. (7), an equation for the isobaric ideal gas heat capacity is required. Ethanol has 21 vibrational frequencies. There are several sources that report vibrational wave numbers including Green [45], Brickwedde et al. [41], and Barrow [46]. Even though these sources were available for the wave numbers, a purely empirical representation was chosen. This was done to reduce the number of terms in the equation. The empirical form used in this work represents the theoretical behavior of the ideal gas heat capacity, and is given by,

$$\frac{c_p^0}{R} = d_1 + \sum_{i=2}^5 d_i \frac{(\theta_i/T)^2 \exp(\theta_i/T)}{[\exp(\theta_i/T) - 1]^2} \quad (8)$$

In Eq. (6),  $d_1 = 6.41129104405$ ,  $d_2 = 1.95988750679$ ,  $d_3 = 7.60084166080$ ,  $d_4 = 3.89583440622$ ,  $d_5 = 4.23238091363$ ,  $\theta_2 = 964$ ,  $\theta_3 = 1549$ ,  $\theta_4 = 2911$ , and  $\theta_5 = 4659$ . These  $d_i$  and  $\theta_i$  values were determined by fitting the functional form of Eq. (8) to the data reported by Brickwedde et al. [41]. Eq. (6) is valid up to 1500 K. Eq. (8) reproduces the Brickwedde et al. [41] data to within  $\pm 0.02\%$ .

The real fluid residual dimensionless Helmholtz energy is given by,

$$\bar{\alpha}(\delta, \tau) = \sum_{k=1}^m N_k \delta^{i_k} \tau^{j_k} \exp(-\gamma \delta^{l_k}) \quad (9)$$

where  $N_k$  are the coefficients of the residual function and  $\gamma$  is set equal to zero (when  $l_k$  is zero) or a value of one (when  $l_k$  is non-zero). The values of  $i_k$ ,  $j_k$ , and  $l_k$  are arbitrary, however it is generally expected that  $i_k$  is an integer,  $j_k$  is a real number, and  $l_k$  is an integer greater than or equal to zero.

An initial comprehensive function containing 100 terms was used to represent Eq. (9). A step-wise linear least squares algorithm incorporating a search procedure based on

statistical parameters was then utilized to determine the final function. The resulting values of  $N_k$ ,  $i_k$ ,  $j_k$ , and  $l_k$  are summarized in Table III. These coefficients and exponents were determined using the data indicated by asterisks in Table I.

The thermodynamic properties of a fluid are determined by differentiation of the fundamental equation. The properties common to engineering design are summarized in the following equations using density and temperature as independent variables.

$$\text{pressure:} \quad P = \rho RT \left[ 1 + \delta \left( \frac{\partial \bar{\alpha}}{\partial \delta} \right)_{\tau} \right] \quad (10)$$

$$\text{internal energy:} \quad u = RT_c \left[ \left( \frac{\partial \alpha^0}{\partial \tau} \right)_{\delta} + \left( \frac{\partial \bar{\alpha}}{\partial \tau} \right)_{\delta} \right] \quad (11)$$

$$\text{enthalpy:} \quad h = RT_c \left[ \left( \frac{\partial \alpha^0}{\partial \tau} \right)_{\delta} + \left( \frac{\partial \bar{\alpha}}{\partial \tau} \right)_{\delta} \right] + \delta \left( \frac{\partial \bar{\alpha}}{\partial \delta} \right)_{\tau} + 1 \quad (12)$$

$$\text{entropy:} \quad s = R\tau \left[ \left( \frac{\partial \alpha^0}{\partial \tau} \right)_{\delta} + \left( \frac{\partial \bar{\alpha}}{\partial \tau} \right)_{\delta} \right] - \alpha^0 - \bar{\alpha} \quad (13)$$

$$\text{isochoric heat capacity:} \quad c_v = -R\tau^2 \left[ \left( \frac{\partial^2 \alpha^0}{\partial \tau^2} \right)_{\delta} + \left( \frac{\partial^2 \bar{\alpha}}{\partial \tau^2} \right)_{\delta} \right] \quad (14)$$

$$\text{isobaric heat capacity:} \quad c_p = c_v + \frac{\left[ 1 + \delta \left( \frac{\partial \bar{\alpha}}{\partial \delta} \right)_{\tau} - \delta \tau \left( \frac{\partial^2 \bar{\alpha}}{\partial \delta \partial \tau} \right) \right]^2}{1 + 2\delta \left( \frac{\partial \bar{\alpha}}{\partial \delta} \right)_{\tau} + \delta^2 \left( \frac{\partial^2 \bar{\alpha}}{\partial \delta^2} \right)_{\tau}} \quad (15)$$

$$\text{velocity of sound:} \quad w^2 = RT \left( \frac{c_p}{c_v} \right) \left[ 1 + 2\delta \left( \frac{\partial \bar{\alpha}}{\partial \delta} \right)_{\tau} + \delta^2 \left( \frac{\partial^2 \bar{\alpha}}{\partial \delta^2} \right)_{\tau} \right] \quad (16)$$

All of the data forms marked with an asterisk in Table 1 were fit simultaneously, thus ensuring proper slope and curvature behavior of the fundamental equation. This



multi-property fitting procedure provides for thermodynamically consistent property calculation from the fundamental equation.

## **5. ACCURACY ASSESSMENT OF THE FUNDAMENTAL EQUATION**

The accuracy of the fundamental equation was determined by statistical comparisons (both graphical and tabular) of property values calculated with the fundamental equation to experimental data. The percent deviation in any property,  $X$ , given by Eq. (2), forms the basis for graphical comparisons. Deviation plots showing percent deviation in density, heat capacity, and velocity of sound were constructed and reviewed to assess the accuracy of the fundamental equation. The tabular results of the statistical analyses are summarized in Tables I and II in the AAD columns. The AAD is the absolute average deviation of any property,  $X$ , defined by Eq. (1). In Table I, the AAD is computed for all data. Asterisks indicate those data used to develop the fundamental equation. In Table II, there are two AAD columns. The first column indicates the AAD for the property computed directly from the fundamental equation by invoking the Maxwell Criterion. The second column is the AAD for the property computed from the ancillary equations. In the case of the ideal gas heat capacity, the AAD is based upon values computed from Eq. (6).

Even though the single-phase data extend to a low temperature of 193 K, the lowest temperature for the saturation data is 273 K. The lack of saturation data below 273 K, particularly vapor pressure data, makes extrapolation somewhat uncertain. The form of the vapor pressure equation used in this work is based on the well-known

Wagner form, and is fairly simple; possessing only four terms. Because of this, the authors feel comfortable declaring a lower limit of 250 K on this formulation.

The upper temperature limit of the formulation (650 K) is a slight extrapolation beyond the the vapor phase data of Bich et al. [1]. The data of Tammann and Ruhenbeck [15] extends to 673 K, but was found to be inconsistent with other data. The upper limit in pressure is 280 MPa, based on the velocity of sound data of Sun et al. [13]. The data of Hawley et al. [4] extends to 479 MPa, and is represented by the fundamental equation, but these eight data points are on one isotherm (303 K).

Based upon the statistical analysis (both graphical and tabular), the authors feel that the formulation presented here can be used to compute the thermodynamic properties of ethanol to within  $\pm 0.2\%$  in density,  $\pm 3\%$  in heat capacity, and  $\pm 1\%$  in velocity of sound. Saturation values of the vapor pressure and saturation densities are represented by the fundamental equation to within  $\pm 0.5\%$ , except near the critical point.

An indication of the qualitative accuracy of any equation of state can be seen in property plots. In plots like these, it is easy to pick out uncharacteristic behavior. Figure 1 shows a plot of isobaric heat capacity versus temperature with several isobars included. This figure shows correct physical behavior of this property, an indication that the first derivative properties, such as internal energy, enthalpy, and entropy, may be considered to be reliable.

## 6. CONCLUSIONS

The fundamental equation presented in this paper represents the current state of the art concerning the thermodynamic properties of ethanol. While this equation can be

used with confidence to compute thermodynamic properties of ethanol in the specified range, this equation can be improved on with additional experimental data.

In general, further measurements of the thermodynamic properties of ethanol are required to both extend the range of the equation, and to improve the accuracy of the heat capacity calculations.  $P$ - $\rho$ - $T$  measurements in the vapor phase, to accompany the data of Bich et al. [1] would be helpful in extending the equation to higher temperatures. An intensive experimental study of the isochoric heat capacity, especially in the liquid phase, would be very helpful to improve the accuracy of the heat capacity calculation.

Saturation data, especially low-temperature vapor pressure and saturated vapor density, along with saturation heat capacity are needed to bring the low-temperature limit of the fundamental equation to be consistent with the low-temperature velocity of sound data of Sun et al. [13].

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**Table I**  
*Single Phase Data for Ethanol*

Reference	Points	Pressure (MPa)		Temperature (K)		AAD
		min	max	min	max	
<b>Pressure-Density-Temperature</b>						
*Bich et al. [1]	34	0.04	0.17	348	631	0.071
Golubev et al. [2]	106	1.00	50.00	200	570	0.620
Gupta and Hanks [3]	24	2.76	22.06	273	363	0.067
Hawley et al. [4]	8	0.10	478.76	303	303	0.161
Hilczer and Goc [5]	6	8.11	44.58	298	298	0.322
Hu et al. [6]	5	0.10	0.10	298	303	0.059
Kalafati [7]	216	0.87	21.47	423	573	8.829
Kubota et al. [8]	46	0.10	310.40	298	323	0.307
*Lo and Stiel [9]	162	8.27	68.95	473	623	0.286
Nikam et al. [10]	5	0.10	0.10	298	313	0.067
Ozawa et al. [11]	41	9.90	196.20	298	348	0.083
*Sauermann et al. [12]	97	0.10	56.70	263	483	0.079
Sun et al. [13]	120	0.10	280.00	193	263	0.153
*Takaguchi and Uematsu [14]	116	0.02	200.01	310	363	0.059
Tammann and Ruhenbeck [15]	113	0.04	96.52	293	673	8.900
Tanyam [16]	44	7.01	310.38	298	323	0.315
Tu et al. [17]	3	0.10	0.10	298	318	0.036
Wilson et al. [18]	65	0.06	0.39	373	473	0.627
<b>TOTAL</b>	<b>1211</b>	<b>0.02</b>	<b>478.76</b>	<b>193</b>	<b>673</b>	
<b>Isobaric Heat Capacity (Cp)</b>						
Counsell et al. [19]	25	0.03	0.10	330	475	6.746
Dong et al. [20]	24	0.03	0.10	331	424	8.811
Pedersen et al. [21]	16	0.10	0.10	301	344	5.626
Sinke and DeVries [22]	9	0.10	0.10	354	437	7.624
Stromsoe et al. [23]	12	0.10	0.10	357	651	8.000
Sun et al. [13]	120	0.10	280.00	193	263	2.759
<b>TOTAL</b>	<b>206</b>	<b>0.03</b>	<b>280.00</b>	<b>193</b>	<b>651</b>	
<b>Isochoric Heat Capacity (Cv)</b>						
Sun et al.	120	0.10	280.00	193	263	3.048
<b>Velocity of Sound</b>						
Carnevale and Litovitz [24]	5	0.10	196.13	303	303	0.671
Eden and Richardson [25]	3	0.00	98.07	293	293	2.817
Hawley et al. [4]	8	0.10	478.76	303	479	1.383
*Sun et al. [13]	120	0.10	275.93	193	263	0.663
*Wilson and Bradley [26]	48	0.10	96.53	273	323	0.924
<b>TOTAL</b>	<b>184</b>	<b>0.00</b>	<b>478.8</b>	<b>193</b>	<b>479</b>	

\*Data used in correlation procedures.

**Table II**  
*Saturation Data and Ideal Gas Heat Capacity Data for Ethanol*

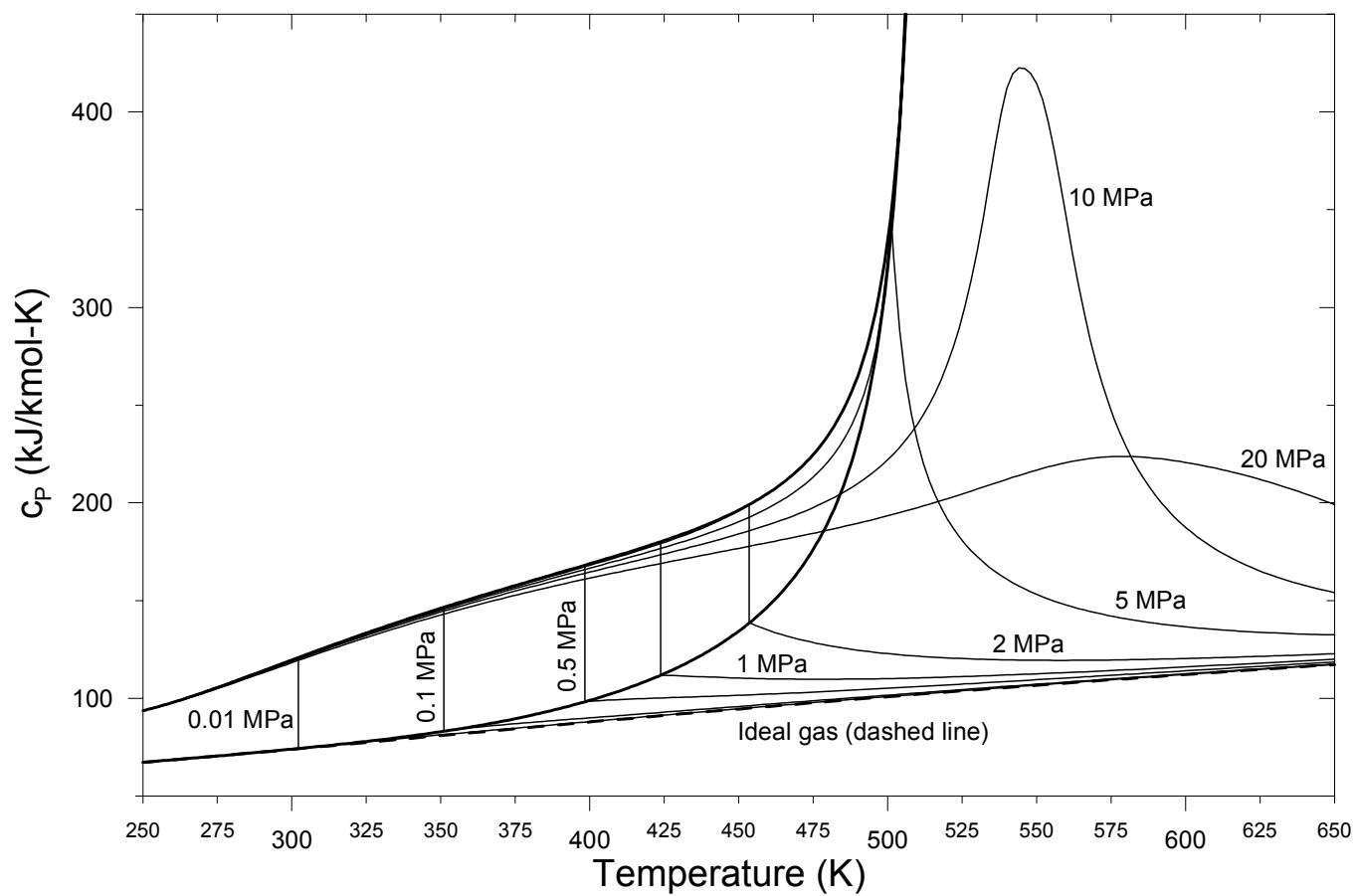
<b>Vapor Pressure</b>		Pressure (MPa)		Temperature (K)		AAD	
Reference	Points	min	max	min	max	Fund Eq	Eq. (1)
*Ambrose and Sprake [27]	25	0.006	0.179	293	367	0.439	0.029
*Ambrose et al. [28]	23	0.168	6.148	365	514	0.412	0.051
Aucejo et al. [29]	22	0.030	0.130	324	358	0.694	0.451
Dulitskaya [30]	3	0.008	0.089	298	348	0.703	0.234
Figurski and Malanowski [31]	17	0.013	0.098	307	351	0.515	0.089
Khurma et al. [32]	3	0.008	0.505	298	399	0.240	0.242
*Kretschmer and Wiebe [33]	8	0.002	0.102	273	352	0.697	0.112
Lee and Hu [34]	6	0.075	0.159	344	363	0.129	0.132
Lydersen and Tsochev [35]	12	2.660	6.165	469	515	2.439	1.651
Mischienko and Subbotina [36]	22	0.002	0.024	277	319	1.065	0.283
Mousa [37]	33	0.020	6.325	319	516	5.793	5.362
Sauermann et al. [12]	21	0.048	2.959	334	473	0.299	0.072
<b>TOTAL</b>	<b>195</b>	<b>0.002</b>	<b>6.325</b>	<b>273</b>	<b>516</b>		
<b>Saturated Liquid Density</b>		Density (mol·dm <sup>-3</sup> )		Temperature (K)		AAD	
Reference	Points	min	max	min	max	Fund Eq	Eq. (2)
Fiock et al. [38]	14	15.0	17.5	273	393	0.135	0.085
*Golick et al. [39]	8	15.7	17.1	293	363	0.039	0.019
*Hales and Ellender [40]	13	12.9	17.1	293	455	0.089	0.011
Mousa [37]	16	5.9	15.0	417	516	10.985	11.506
<b>TOTAL</b>	<b>51</b>	<b>5.9</b>	<b>17.5</b>	<b>273</b>	<b>516</b>		
<b>Saturated Vapor Density</b>		Density (mol·dm <sup>-3</sup> )		Temperature (K)		AAD	
Reference	Points	min	max	min	max	Fund Eq	Eq. (3)
*Fiock et al. [38]	14	0.001	0.145	273	393	1.426	0.236
Mousa [37]	16	0.653	5.917	417	516	19.165	17.610
<b>TOTAL</b>	<b>30</b>	<b>0.001</b>	<b>5.917</b>	<b>273</b>	<b>516</b>		
<b>Ideal Gas Heat Capacity</b>		$c_p^0$ (J·mol <sup>-1</sup> ·K <sup>-1</sup> )		Temperature (K)		AAD	
Reference	Points	min	max	min	max	Fund Eq	Eq. (6)
*Brickwedde et al. [41]	14	73.6	167.7	298	1499	-	0.012

\*Data used in correlation procedures.

**Table III**  
*Coefficients and Exponents of the Fundamental Equation for Ethanol*

$N_k$	$i_k$	$j_k$	$l_k$
$1.14008942201 \times 10^1$	1	-0.5	0
$-3.95227128302 \times 10^1$	1	0	0
$4.13063408370 \times 10^1$	1	0.5	0
$-1.88892923721 \times 10^1$	1	1.5	0
$4.72310314140$	1	2	0
$-7.78322827052 \times 10^{-3}$	1	5	0
$1.71707850032 \times 10^{-1}$	2	-0.5	0
$-1.53758307602$	2	1	0
$1.42405508571$	2	2	0
$1.32732097050 \times 10^{-1}$	3	0	0
$-1.14231649761 \times 10^{-1}$	3	2.5	0
$3.27686088736 \times 10^{-6}$	6	6	0
$4.95699527725 \times 10^{-4}$	7	2	0
$-7.01090149558 \times 10^{-5}$	8	2	0
$-2.25019381648 \times 10^{-6}$	8	4	0
$-2.55406026981 \times 10^{-1}$	1	5	2
$-6.32036870646 \times 10^{-2}$	3	3	2
$-3.14882729522 \times 10^{-2}$	3	7	2
$2.56187828185 \times 10^{-2}$	6	5.5	2
$-3.08694499382 \times 10^{-2}$	7	4	2
$7.22046283076 \times 10^{-3}$	8	1	2
$2.99286406225 \times 10^{-3}$	2	22	4
$9.72795913095 \times 10^{-4}$	7	23	4





**Figure 1.**  $c_p$ - $T$  plot for ethanol computed from the fundamental equation